Triethylenetetramine

112-24-3 | DTXSID9023702

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 16.4 °C

Global applicability domain: Outside

Local applicability domain index: 3.54e-01

Confidence level: 3.31e-01

Nearest Neighbors from the Training Set

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Triethylenetetramine
Measured: 12.0
Predicted: 16.4

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1,4-Butanediamine, N,N'-bis(3-aminopropyl)-
Measured: 29.0
Predicted: 35.0

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Tetraethylenepentamine
Measured: -30.0
Predicted: -12.9

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Diethylenetriamine
Measured: -39.0
Predicted: -35.3

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Cyclam
Measured: 185
Predicted: 157